OFFICE OF THE
SCIENCE ADVISOR

GUIDANCE

CHAPTER 5

Selection, Use and Limitations of Indicator Chemicals for Evaluation of Exposure to Complex Waste Mixtures

ABSTRACT

Quantitative evaluation of all chemicals of potential concern is the most thorough approach for assessing potential health risks posed by exposures to chemicals emanating from hazardous waste sites and permitted facilities. Utilization of computer spreadsheet programs facilitates carrying all chemicals of potential concern through the risk assessment. It is expected most quantitative risk assessments of hazardous waste sites and permitted facilities will evaluate all chemicals of potential concern. However, for certain sites or facilities, the list of potentially site-related chemicals remaining after quantitation limits, qualifiers, blank contamination and background have been evaluated may exceed a manageable number. In other instances, there may be a number of individual chemicals for which toxicity data and/or health-based criteria are not available. In such cases, it is reasonable to use an indicator chemical approach to provide an estimate of the potential health risks associated with exposure to these substances.

Chemicals accounting for at least 95% of the risk are to be considered in the comprehensive risk assessment. As discussed in this document, chemicals should not be eliminated from evaluation if they possess certain types of toxicity or toxic potency, e.g., known human carcinogens. The indicator chemical should be similar in terms of environmental fate, transport, persistence, and inherent toxicity to the chemicals it is to represent, and should not be used for special environmental routes, such as the food pathway exposure route. Examples of how to determine chemical class, and how to select indicator chemicals, are provided in this document. It should be recognized that the indicator chemical approach requires a significant expenditure of time and effort to implement and to justify and may exceed the time needed to simply carry all chemicals of potential concern through a comprehensive quantitative risk assessment.

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1 INTRODUCTION

1.1 Purpose

1.1.1 Necessity

Quantitative evaluation of all chemicals of potential concern is the most thorough approach for assessing potential health risks posed by exposures to chemicals emanating from hazardous waste sites and permitted facilities. Utilization of computer spreadsheet programs facilitates carrying all chemicals of potential concern through the risk assessment. It is expected most quantitative risk assessments of hazardous waste sites and permitted facilities will evaluate all chemicals of potential concern. However, for certain sites or facilities, the list of potentially site-related chemicals remaining after quantitation limits, qualifiers, blank contamination, and background have been evaluated may exceed a manageable number (i.e., greater than 25). In other instances there may be a number of individual chemicals for which toxicity data and/or health-based criteria are not available. In such cases it is reasonable to use an indicator chemical approach to provide an estimate of the potential health risks associated with exposure to these substances.

It is important to recognize that the time required to implement and justify the indicator chemical selection procedures detailed in this document may exceed the time needed to simply carry all the chemicals of potential concern through a comprehensive quantitative risk assessment. Therefore, it is anticipated that the procedures described in this document may be necessary only for the most complex hazardous waste sites and facilities or only for specific chemical waste mixtures.

1.1.2 Regulatory Context

The guidance provided in this document is intended to be consistent with the U. S. Environmental Protection Agency's (EPA's) Risk Assessment Guidance for Superfund, Volume I, Health Evaluation Manual (Part A), Interim Final (EPA/540/1-89/002, December 1989).

Currently, EPA requires that risk assessments of hazardous waste sites and permitted facilities follow the process and procedures described in the above referenced document.

1.2 Application

1.2.1 How and When Guidance Should be Used

This guidance is designed to provide information that will assist in the development of a quantitative human health risk assessment for a hazardous waste site or a permitted facility. The approach for selection of indicator chemicals for complex waste mixtures may or may not be adopted for a particular site or facility, depending on what is reasonable and appropriate for the facility and what is required by the Department of Toxic Substances Control (DTSC) toxicologists . Therefore, DTSC officials may decide to follow the guidance provided in this document, or to act at variance with the guidance, based on analysis of the individual, site-specific characteristics of the facility being evaluated. In general, since the indicator chemical approach requires a significant expenditure of time and effort to develop and justify, only complex sites or facilities that involve a substantial number of individual chemicals (i.e., greater than 25) will benefit from using this method. For this reason, the approach described herein should not be considered "simplified."

This document is intended to be used in conjunction with other guidance reports prepared by DTSC and the U. S. EPA, in particular the EPA's Risk Assessment Guidance for Superfund, Volume I, Human Health Evaluation Manual (Part A), (U. S. EPA 1989).

1.2.2 Who Should Use This Guidance

This guidance document is addressed primarily to individuals who conduct human health risk assessments for hazardous waste sites or facilities. It is also targeted to DTSC staff responsible for review and oversight of human health risk assessments. Officials at the federal, state, and local level who are involved in the remediation of hazardous waste sites and/or the permitting of facilities that handle hazardous wastes may also benefit from this guidance.

1.2.3 Major Points of the Guidance

This report provides specific guidance for reducing the number of individual chemicals that are included in a quantitative assessment of human health risk for exposure to chemicals originating from a

hazardous waste site or permitted facility. The primary aspects of this guidance are:

- Known human carcinogens (i.e., classified by the U. S. EPA in weight-of-evidence Group A, or by International Agency for Research on Cancer (IARC) in Group I), known human developmental toxins, and known human reproductive toxins may not be eliminated from a quantitative human health risk assessment, even if the indicator chemical selection procedure indicates that such elimination is justified.

- Justification for selection of surrogate chemicals should include qualitative or quantitative consideration of environmental mobility, persistence, and bioaccumulation.

- In general, the indicator chemical procedure should not be employed to eliminate essential elements or toxic metals from consideration in a human health risk assessment.

- All chemicals detected at the site or facility being evaluated should be grouped into classes that reflect similarity of chemical structure.

- The toxicity of chemicals that either (a) lack a toxic potency value, or (b) are poorly identified or identified only by generic description (e.g., "unidentified glycol ethers"), is assumed to be equivalent to the toxicity of the most toxic member of the same chemical class.

- To identify a set of indicator chemicals, each chemical is ranked by calculating an arithmetic expression that accounts for toxicity, concentration in each medium of exposure, and the toxicity and concentration of all the chemicals detected at the facility. Each chemical class must be represented by at least one chemical (i.e., this procedure cannot be used to eliminate entire classes of chemicals). Carcinogens and noncarcinogens are evaluated in separate analyses. This procedure is intended to ensure that chemicals accounting for at least 95 percent of the risk associated with a facility are considered in the comprehensive risk assessment.

1.3 LIMITATIONS

It is important to recognize that the time required to implement and justify the indicator chemical selection procedures detailed in this guidance document may exceed the time needed to simply carry all of the chemicals

of potential concern through a comprehensive quantitative risk assessment. Therefore, it is anticipated that the procedures described in this document may be applicable only for the most complex hazardous waste sites and facilities or only for specific chemical waste mixtures.

2 METHODS

2.1 CONSULTATION WITH THE DTSC

The purpose of a quantitative risk assessment of a hazardous waste site or permitted facility is to provide a reasonable upper bound estimate of the potential health risks associated with exposures to chemicals emanating from such facilities. The results of a quantitative risk assessment are used in part for, and indeed may be the basis for justification of, a risk management decision concerning remedial or control measures at the site or facility. Therefore, it is necessary that a risk assessment be accurate and thorough, and that all potential chemical exposures be evaluated. Since elimination of potential chemicals of concern from consideration in a risk assessment could lead to underestimation of the potential health threats posed by chemicals emitted from the site or facility, it is prudent and in the best interest of DTSC and the citizens of California for DTSC to review any and all proposals by interested parties to eliminate from consideration any chemicals of potential concern from a quantitative risk assessment. Written approval by a DTSC toxicologist or project manager must be obtained prior to DTSC sanction of the elimination of chemicals of potential concern from consideration in a risk assessment. The DTSC toxicologist's review and evaluation shall be in writing, and form a portion of the available public record, and shall include a scientifically supported expert opinion as to whether or not each such proposal is scientifically based, adequately justified, and likely to result in a significant underestimation of the potential health risks posed by the site or facility. In general, this review will be completed within six weeks from receipt of the proposal by the Toxicology and Risk Assessment Section.

2.2 DOCUMENTATION OF THE RATIONALE FOR ELIMINATING CHEMICALS OF CONCERN FROM CONSIDERATION IN THE RISK ASSESSMENT

Since the risk assessment report is a part of the public record, and contributes to DTSC's or the interested party's risk management decision, it is necessary that a list of all chemicals eliminated from consideration from a risk assessment and the rationale for eliminating these chemicals from the

quantitative risk assessment, based upon the procedures detailed in this guidance document, be clearly stated in the main body of the risk assessment report.

2.3 HISTORICAL SITE-SPECIFIC USE INFORMATION

Historical data concerning chemicals, waste processes, etc., associated with site activities often provide important information concerning the types of, and possible sources for, contaminant releases into the environment. A quantitative risk assessment should be a comprehensive document that addresses the potential health threats associated with chemicals associated with both current and past hazardous waste generation, storage , and disposal procedures. However, it is acceptable to eliminate from consideration in the quantitative risk assessment chemicals historically associated with site or facility activities if the indicator chemical selection procedures outlined in this guidance document shows that such an elimination is justified.

2.4 KNOWN HUMAN CARCINOGENS

The classification of a chemical by EPA or by the IARC as a known human carcinogen means that these organizations have concluded that epidemiological scientific evidence clearly shows a causal association between exposure to these substances and the development of cancer in humans. Therefore, there is a clear human health threat when humans are exposed to these substances, and a quantitative risk assessment of a hazardous waste site or facility emitting such substances into the environment must address the potential human health threats posed by these substances.

DTSC recognizes that both inherent toxicity and exposure are necessary to produce a health risk, even for substances that are known human carcinogens. However, the likelihood that such substances would pose a cancer risk to exposed humans is greater than that for exposures to substances classified as probable or possible carcinogens, based upon experimental observations in laboratory animals. To ensure that the potential health risks posed by those substances most likely to adversely affect human health are not eliminated from evaluation in a quantitative risk assessment, to meet the concerns of the public regarding risks posed by known human carcinogens, and to provide the risk manager with sufficient human health risk information to make an informed decision, known human carcinogens (EPA Group A, IARC Group 1) should not be eliminated from evaluation in a quantitative risk assessment even if the indicator selection procedures indicate such an elimination is possible.

2.5 KNOWN HUMAN DEVELOPMENTAL AND REPRODUCTIVE TOXINS

The classification of a chemical known to be a human reproductive or developmental toxin is based upon epidemiological scientific evidence that clearly shows a causal association between exposure to these substances and the production of developmental or reproductive toxicities in humans. Therefore, there is a clear threat to human health when humans are exposed to these substances, and a quantitative risk assessment of a hazardous waste site or facility emitting such substances into the environment must address the potential human health threats posed by these substances.

DTSC recognizes that both inherent toxicity and exposure are necessary to produce a health risk, even for substances that are known human reproductive and developmental toxins. However, the likelihood that such substances would pose a health threat to exposed humans is greater than that for exposures to substances classified as reproductive or developmental toxins, based solely upon experimental observations in laboratory animals. To ensure that the potential health risks posed by those substances most likely to adversely affect human health are not eliminated from evaluation in a quantitative risk assessment, and to meet the concerns of the public regarding risks posed by known human reproductive and developmental toxins, and to provide the risk manager with sufficient human health risk information to make an informed decision, known human reproductive and developmental toxins should not be eliminated from evaluation in a quantitative risk assessment even if the indicator selection procedures indicate such an elimination is possible.

2.6 MOBILITY, PERSISTENCE, AND BIOACCUMULATION AND ECOLOGICAL EFFECTS

Exposure to chemicals contaminating a hazardous waste site or facility is governed by a complex interplay of chemical specific physio-chemical parameters and site-specific characteristics. The potential for human exposure to such hazardous chemicals is dependent, in part, upon the fate, transport, and/or persistence of these substances in environmental media, or bioconcentration in flora or fauna. The procedures detailed in this document for the selection of indicator chemicals do not explicitly include a component to assess environmental fate, transport, and persistence of hazardous waste chemicals. Therefore, it is necessary to apply scientific judgment, as well as the objective criteria detailed in this document, in the selection of indicator chemicals to ensure that substances that are highly mobile in the environment, substances that are highly persistent in the environment, and substances that are highly bioconcentrated are not eliminated from consideration in the risk assessment. The actual human health risks posed by such substances may not be fully appreciated during

initial evaluations, yet, due to environmental transport, persistence or bioconcentration of such substances, humans may ultimately be exposed to these substances at a much larger level than would be estimated by simply evaluating concentration and toxicity data alone. The main body of the risk assessment report shall include a qualitative or quantitative evaluation of mobility, persistence and bioaccumulation in relation to the selection of indicator chemicals. For each indicator chemical chosen, written justification shall be provided to document that environmental fate, transport, persistence, bioaccumulation, ecological effects were evaluated in the selection process.

The intent of this recommendation is to ensure that consideration is given to substances that may migrate in the environment and to substances that are highly bioconcentrated since the actual human health risks posed by such contaminants may not be fully appreciated during initial site evaluations. For such substances, in particular, chemicals which are bioconcentrated in food stuffs, fish, shellfish, or livestock, humans could be exposed to a much larger extent than would be estimated based upon intakes of air, water, and soil. It is also of importance to consider environmental fate when evaluating soil and ground water contaminants, since it is possible that, at the time of investigation, significant concentrations may not be present in ground water, but could reasonably be expected to migrate into ground water prior to effective remediation of the contaminated soil.

2.7 SPECIAL EXPOSURE ROUTES

The indicator chemicals selected according to the procedures outlined in this guidance may not be applicable to assessing ecological threats or for assessing health threats from the food pathway or for assessing threats due to volatilization from contaminated household water into indoor air. Therefore, the indicator chemical procedure should not be used for special exposure routes (e.g., the food pathway exposure route, volatilization into indoor air from household water, etc.).

2.8 GROUPING CHEMICALS BY CLASS

Some examples of appropriate chemical classes (and members of these classes) that are commonly associated with hazardous waste sites and permitted facilities are included in Appendix A. Neither the chemical classes nor the members of each class are to be taken as comprehensive. Rather, this information is provided only for illustrative purposes. Selection of chemical classes should be consistent with the logic of this list, and, in addition, it may be beneficial to also consider environmental fate and transport considerations when grouping chemicals.

If a chemical is to be chosen as an indicator chemical to represent several

chemicals, then the indicator chemical should be similar in terms of environmental fate, transport, persistence and inherent toxicity of the chemicals it is to represent. In many, but not all cases, chemicals with similar structures are likely to exhibit similar physio-chemical properties and similar toxicities. Therefore, the chemicals contaminating a particular medium are first grouped according to chemical class, so that an indicator chemical (or if necessary, several indicator chemicals) can be chosen to represent each and every class of chemical contaminants.

Separately, for each medium (air, water, soil), all of the chemicals detected at the site/facility should be grouped into classes based upon chemical structure, chemical class, or other chemical similarities.

Do not group solely by toxicity characteristics.

Do not group all carcinogenic or all noncarcinogenic chemicals without regard to chemical class, structure, or other chemical similarities.

Do not group chemicals by analytic techniques or physio-chemical properties (i.e., do not group chemicals into the classes of volatile organic compounds or semi-volatile organic compounds).

2.9 EVALUATION OF THE FREQUENCY OF DETECTION OF EACH CHEMICAL

Chemicals that are infrequently detected may be artifacts in the data due to sampling, analytical, or other problems, and therefore may not be related to site operations or disposal practices. Consider the chemical as a candidate for elimination from the quantitative risk assessment if it meets the criteria for a laboratory contaminant as specified in the EPA Risk Assessment Guidance for Superfund, Human Health Evaluation Manual, December 1989.

Available modeling results may indicate whether monitoring data that show infrequently detected chemicals are representative of only their sampling locations or of broader areas. Because chemical concentrations at a site are spatially variable, the risk assessor can use modeling results to project infrequently detected chemical concentrations over broader areas when determining whether the subject chemicals are relevant to the overall risk assessment. In general, when only limited characterization data is available (e.g., less than 20 samples per medium), it is inappropriate to eliminate infrequently detected chemicals. For the extensively characterized site or facility, any detection frequency limit to be used (e.g., five percent) as justification for elimination of infrequently detected chemicals should be approved by a DTSC toxicologist or site manager.

In addition to available monitoring data and modeling results, the risk assessor will need to consider other relevant factors (e.g., presence of sensitive subpopulations) in recommending appropriate site-specific limits on inclusion of infrequently detected chemicals in the quantitative risk assessment. For example, the risk assessor should consider whether the chemical is expected to be present based on historical data or any other relevant information (e.g., known degradation products of chemicals present at the site, modeling results). Chemicals expected to be present should not be eliminated based on their low frequency of detection.

For some chemicals the sample quantitation limits may exceed the concentration of concern for potential adverse health effects. Examples include benzene and vinyl chloride. In such cases it may be necessary to utilize more sensitive analytical techniques, or alternatively, assume that the chemicals of potential concern are present but at some level below the sample quantitation limit. For further guidance, refer to the DTSC guidance document on use of concentration data and to EPA Risk Assessment Guidance for Superfund, December 1989.

The reported or modeled concentrations and locations of chemicals should be evaluated to determine if the distribution "hotspot" should not be eliminated from the risk assessment. Always consider detection of particular chemicals in all sampled media because some media may be sources of contamination for other media. For example, a chemical that is infrequently detected in soil (a potential ground water contamination source) probably should not be eliminated as a site contaminant if the same chemical is frequently detected in ground water. In addition, infrequently detected chemicals with high concentrations should not be eliminated.

Therefore, for each chemical in each medium (air, water, soil) document frequency of detection data, and evaluate such data to determine if infrequently detected substances could be artifacts due to problems associated with sampling or analysis or other procedures.

2.10 EVALUATION OF ESSENTIAL ELEMENTS

Essential elements, defined as essential human nutrients and toxic only at very high doses (i.e., much higher than those that could be associated with contact at the site) should be candidates for elimination from a quantitative risk assessment of a hazardous waste site or permitted facility. Examples of such chemicals are iron, magnesium, calcium, potassium, sodium, and zinc. Essential elements that should not be eliminated from consideration include arsenic, selenium, copper, and chromium, since these metals pose a significantly greater risk to health and the environment.

Prior to eliminating essential elements from the risk assessment, they must

be shown to be present at levels that are not likely to be associated with adverse health effects. The determination of acceptable dietary levels for these substances is often very difficult. Literature values concerning acceptable dietary levels may conflict and may change fairly often as new studies are conducted. For example, arsenic--a known human carcinogen--is considered by some scientists to be an essential nutrient based on animal experiments; however, acceptable dietary levels, if any, are not known for humans. Therefore, arsenic should be retained in the risk assessment. Another example is chromium. Chromium (III) is considered to be an essential nutrient, however, chromium (VI) is considered to pose a carcinogenic risk to humans.

For these reasons, the use of an indicator chemical approach for essential elements is not recommended.

In summary, the use of an indicator chemical approach for essential elements is generally not acceptable since the toxicity characteristics of each element are unique and it is therefore difficult, if not impossible, to quantitatively approximate the total potential risk of all essential elements by use of an indicator element.

2.11 EVALUATION OF TOXIC METALS

The indicator chemical approach for toxic metals is not recommended. Toxic metals include some essential elements, such as arsenic and chromium, as well as such nonessential elements as vanadium, beryllium, and barium. Such toxic metals should not be eliminated from consideration in the quantitative risk assessment unless the concentrations can be shown to be equivalent to naturally occurring levels. For guidance in determining background concentrations of toxic metals refer to EPA Risk Assessment Guidance for Superfund, Human Health Evaluation Manual, Chapter 5. Note that in some cases, background concentrations may present a significant risk, and while cleanup may or may not eliminate this risk, it may be necessary to evaluate background risk to provide important information to the affected public and to risk managers. If background concentrations of inorganic substances pose significant risks, then it is suggested that the quantitative risk assessment present risk estimates for the risks associated with exposure to the background concentration, the site concentration, and the total concentration.

2.12 SELECTION OF AN INDICATOR CHEMICAL FOR A CHEMICAL THAT IS INADEQUATELY IDENTIFIED OR THAT LACKS RELEVANT TOXICITY CRITERIA

For some chemicals a toxicity value may not be available from either Cal-EPA or EPA, and in some instances the analytical characterization of the chemical contaminants may be incomplete. In such cases, it is necessary to assume that the toxicity of these compounds were equivalent to the most toxic chemical within the chemical class for which the compound(s) of concern is a member. The toxicity value of the most toxic chemical within the class shall be used, for both the indicator selection procedure and for subsequent quantitative risk assessments, irrespective of the presence or absence of this most toxic chemical in the media of concern.

For example, for chemicals that are poorly identified (e.g., "unidentified glycol ethers") and for chemicals for which entirely health-based criteria are not available (e.g., 1-(2-methoxy-1-methylethoxy)-2)-1-methylethoxy)-2-propanol) it is necessary to consider these substances as if their toxicity were equivalent to the most toxic glycol ether, 2-methoxyethanol acetate. The toxicity value for 2-methoxyethanol acetate should be used initially for the indicator chemical selection procedure. If, using the indicator chemical selection procedure, the compounds(s) described as "unidentified glycol ethers" is selected as an indicator chemical for a subsequent risk assessment, then the toxicity value for 2-methoxyethanol acetate should be used in the quantitative risk assessment to calculate potential human health effects associated with exposure to the compound(s) described as "unidentified glycol ethers".

2.13 EVALUATION OF CHEMICALS OF POTENTIAL CONCERN USING A CONCENTRATION-TOXICITY SCREENING PROCEDURE

The aim of this screening procedure is to identify, using an objective, readily verifiable, arithmetic procedure, those chemicals in a particular medium that based on concentration and toxicity, are most likely to contribute significantly to potential human health threats as a result of exposure to the contaminated medium. Once this has been accomplished, indicator chemicals can be chosen such that it is highly probable that those chemicals eliminated from consideration in the quantitative risk assessment will not pose a significant risk.

The Individual Indicator Chemical Score (IICS), Total Indicator Chemical Score for Carcinogens (TICSC), Total Indicator Chemical Score for Noncarcinogens (TICSN), and associated ratios) parameters developed for the indicator chemical selection procedure are to be used solely for the potential reduction of the number of chemicals carried through a risk assessment of a hazardous waste site or facility. They have no meaning

outside the context of this procedure, and they should not be considered as a quantitative measure to judge a chemical's toxicity or risk to humans, or as a substitute for a formal risk assessment.

2.13.1 Evaluation Procedure

Step 1: Identify the particular chemicals in each medium that--based upon concentration and toxicity--are likely to significantly contribute to the potential health risks associated with exposure to each medium. (An example is included in Appendix B)

For each class of chemicals in each medium, divide the chemicals detected into carcinogens and noncarcinogens. For the purposes of this evaluation carcinogens are defined as substances classified by EPA as "known human carcinogens", "probable human carcinogens", and "possible human carcinogens"; compounds classified by the IARC as "carcinogenic to humans", "probably carcinogenic to humans", and "possibly carcinogenic to humans", compounds classified by DTSC as carcinogens; compounds classified by DHS-Health Hazard Assessment Division as carcinogens; and compounds listed as carcinogens under Proposition 65 regulations.

This is necessary so that the indicator chemicals chosen reflect the potential of the chemical contaminants to cause both systemic toxicity and carcinogenicity. Two of the most important factors when determining the potential effect of excluding a chemical in the risk assessment are its measured concentrations at the site and its toxicity.

Calculate an Individual Indicator Chemical Score (IICS) for each chemical in each medium.

where:

Cij = Concentration of chemical i in medium j; the concentration units must be mg/vol. of medium for air and water, and mg/kg for soil.

Tij = Toxicity value for chemical i
(mg/kg/day)-1

The concentration of each chemical shall be the maximum detected concentration in each medium, irrespective of the sample depth (soil) or whether or not the aquifer is considered to be of current or future beneficial use (water). Concentration shall be expressed in

units of mg/liter for water, mg/m3 for air, and mg/kg for soil.

Each chemical in a medium is then scored according to its concentration and toxicity to obtain an IICS. In obtaining the IICS, the concentration to be used is the maximum concentration of the chemical detected in the medium. This step simplifies the analysis, eliminates the need to consider bias sampling, and also ensures that chemicals of concern are not eliminated due solely to variability in their horizontal or vertical distribution in the medium.

To calculate Tij from a Reference Dose (RfD)

$$Tij = \frac{1}{RfD}$$

To calculate Tij from a Cancer Potency Slope (CPS).

Tij = CPS

The hierarchy for selection of the appropriate Tij to use when a given chemical has more than one health criteria shall be, in order of preference:

A. Cancer potency slope factors or reference doses promulgated into California regulations.

B. Cancer potency slope factors or reference doses used to develop environmental criteria promulgated into California regulations. Examples include cancer potency slope factors or reference doses used in deriving State drinking water Maximum Contaminant Levels (MCL) and cancer potency slope factors used in deriving "no significant risk levels" under the State's Safe Drinking Water and Toxic Enforcement Act of 1986 (Prop 65) . Note: The entirely health-based dose criteria should be used to estimate risk, and not the resulting risk management environmental concentration criteria (the CPS not the MCL).

C. Cancer potency slope factors or reference doses from the U. S. Environmental Protection Agency's Integrated Risk Information System (IRIS).

D. Cancer potency slope factors or reference doses from the U. S. Environmental Protection Agency's Health Effects Assessment Tables (HEAST, the most current edition).

The toxicity values to be used are entirely health-based criteria

derived by Cal-EPA or the EPA (IRIS--Reference Doses or Cancer Potency Factors). Although other criteria from other regulatory programs may be available, they have limited application since they may not be entirely health-based criteria (e.g., State and Federal MCL for drinking water, OSHA Permissible Exposure Limits, ACGIH Threshold Limit Values).

Step 2: Calculate a Total Indicator Chemical Score for Carcinogens (TICSC) for each medium by summing all Individual Indicator Chemical Scores (IICS) for carcinogens.

Once IICSs have been calculated for each chemical in each medium, then the TICSC is calculated for each medium by summing all IICSs for carcinogens separately for each medium.

TICSC(water) = sum IICS(water) for carcinogens

TICSC(air) = sum IICS(air) for carcinogens

TICSC(soil) = sum IICS(soil) for carcinogens

Step 3: Calculate a Total Indicator Chemical Score for Noncarcinogens (TSCSN) for each medium by summing all Individual Indicator Chemical Scores (IICS) for noncarcinogens.

Once IICSs have been calculated for each chemical in each media, then the TICSN is calculated for each medium by summing all IICSs for noncarcinogens separately for each medium.

TICSN(water) = sum IICS(water) for noncarcinogens

TICSN(air) = sum IICS(air) for noncarcinogens

TICSN(soil) = sum IICS(soil) for noncarcinogens

Step 4: For each medium calculate the ratio of the Individual Indicator Chemical Score (IICS) for each carcinogen to the Total Indicator Chemical Score for Carcinogens (TICSC) for the respective medium.

Calculate the value of the IICS for each carcinogenic chemical in each medium divided by the respective media-specific TICSC. The IICS/TICSC ratio provides an approximation of the relative risk for each chemical in each medium.

Step 5: For each medium calculate the ratio of the Individual Indicator Chemical Score (IICS) for each noncarcinogen to the Total Indicator Chemical Score for Noncarcinogens (TICSN) for the respective medium.

Calculate the value of the IICS for each noncarcinogenic chemical in each medium divided by the respective media-specific TICSN. The IICS/TICSN ratio provides an approximation of the relative risk for each chemical in each medium.

Step 6: Select a Set of Indicator Chemicals to be Carried Through a Comprehensive Risk Assessment.

For most hazardous waste sites and permitted facilities it will be necessary to conduct a thorough quantitative risk assessment. If it is desired to use an indicator chemical approach for this comprehensive risk assessment, then indicator chemicals are selected for each medium by selecting a set of indicator carcinogenic and noncarcinogenic chemicals, to include at least one carcinogen and one noncarcinogen from each class, such that the sum of the ratios of the IICS to the TICSC or to the TICSN, as appropriate, for the substances selected is equal to or greater than 0.95. This procedure ensures that only those chemicals that are least likely to produce adverse human health effects are eliminated from consideration in the comprehensive risk assessment. The 0.95 value is designed to ensure that those chemicals responsible for approximately 95 percent of the risks associated with the site are carried through the comprehensive risk assessment. If the quantitative risk assessment reveals that the cancer risk is equal to or exceeds 1 x 10-4 or that the Hazard Index is equal to or exceeds 20, then it may be necessary to review the indicator chemical selection process and augment the set of indicator chemicals with chemicals originally eliminated from consideration.

For each medium select a set of indicator carcinogenic chemicals, to include at least one chemical from each class, such that the sum of the ratios of the IICS to the TICSC for the substances selected is equal to or greater than 0.95.

For each medium select a set of indicator noncarcinogenic chemicals, to include at least one chemical from each class, such that the sum of the ratios of the IICS to the TICSC for the substances selected is equal to or greater than 0.95.

To estimate receptor point exposure concentration for the comprehensive risk assessment, the source term concentration for

each surrogate chemical in each medium shall be the 95 percent upper confidence limit of the arithmetic mean concentration, in accordance with EPA and State guidance.

Since the chemicals selected using the indicator chemical selection procedure are estimated to contribute most significantly to the potential health risks, it may not be necessary to adjust the source term concentrations for the indicators selected to account for the total mass of contaminants. In such cases, the source term concentration for each indicator chemical in each medium should be the 95 percent upper confidence limit of the arithmetic mean concentration of the surrogate chemical, in accordance with EPA guidance (Risk Assessment Guidance for Superfund, Human Health Evaluation manual and DTSC guidance (Guidance Document for Use of Concentration Data).

2.14 DOCUMENTATION OF INDICATOR CHEMICAL SELECTION PROCEDURE

If the indicator chemical approach is utilized, then thorough documentation of the procedure is required to be included in the main body of the risk assessment report. A separate chapter detailing the methodology, calculations, selection of indicators, and supporting justification is desirable.

Whenever possible data should be presented in tabular format. The data shall include a list of all chemicals; chemicals grouped by chemical class; frequency of detection of each chemical in each medium; maximum concentration of each chemical in each medium; the health-based criteria used for the toxicity value (Tij) and a reference as to its source; calculated Individual Indicator Chemical Scores, Total Indicator Chemical Scores, the ratio for each chemical in each medium of the Individual Indicator Chemical Score divided by the appropriate Total Indicator Chemical Score (the risk ratios); the indicator chemicals selected for each medium, their risk ratios, and the sum of their risk ratios.

The discussion of the indicator chemical selection procedure and the justification for selection indicator chemicals shall be in sufficient detail so as to allow for independent verification of the indicator chemical toxicity/concentration selection procedure, and presented in language that is, as far as is feasible, readily understandable to the layman public.

REFERENCES

DTSC. 1992. Department of Toxic Substances Control. Use of Concentration Data In Exposure Assessments. Draft.

IARC. 1987. International Agency for Research on Cancer (IARC) Monographs on the Evaluation of Carcinogenic Risks to Humans. Supplement 7. Overall Evaluations of Carcinogenicity: An updating of IARC Monographs Volumes 1 to 42.

U. S. EPA. Environmental Protection Agency Integrated Risk Information (IRIS). This is a computerized data base which contains toxicity information and toxicity criteria for numerous chemicals. Accessible through MEDLARS.

U. S. EPA. 1989. Risk Assessment Guidance for Superfund Volume 1 Human Health Evaluation Manual (PART A) Interim Final (EPA/540-1-89/002, 1989).

U. S. EPA. 1991. Health Effects Assessment Summary Tables (HEAST).

APPENDICES

Appendix A--Classes of Chemicals and Representative Members of Each Chemical Class

Halogenated C1, C2, and C3 Compounds

Chloroform
Chloromethane
Dichloromethane (Methylene chloride)
Trichlorofluoromethane (Freon 11)
1,1-Dichloroethane
1,2-Dichloroethane (Ethylene dichloride)
1,1,1-Trichloroethane (TCA)
1,1,2-Trichloroethane
Chloroethylene (Vinyl chloride)
1,1-Dichloroethylene (Vinylidene chloride)
cis-1,2,Dichloroethylene
trans-1,2-Dichloroethylene
Trichloroethylene (TCE)
Tetrachloroethylene (Perchloroethylene, PCE)
Carbon Tetrachloride

Ketones

2-Propanone (Acetone)
2-Butanone (Methyl ethyl ketone)
2-Hexanone (Methyl-n-butyl ketone, MNBK)
3,5,5-Trimethyl-2-cyclohexene-1-one (isophorone)

Chlorinated Phenols and Chlorinated Aromatics

Pentachlorophenol
2,4-Dichlorophenol
2,4,5-Trichlorophenol
2 -Chlorophenol
4-Chloro-3-Methylphenol
Chlorobenzene
1,4-Dichlorobenzene

Phthalate Esters and Related Compounds

Di(2-ethylhexyl)phthalate
Butylbenzylphthalate
Di-n-octylphthalate

bis(n-Butyl)phthalate
Di(2-ethylhexyl)phthalate (DEHP)
Di(2-ethylhexyl)adipate (DEHA)

Polychlorinated Dibenzo-p-dioxins and Dibenzofurans

Tetrachlorodibenzo-p-dioxins
Tetrachlorodibenzofurans
Pentachlorinated dibenzo-p-dioxins
Pentachlorinated dibenzofurans
Hexachlorinated dibenzo-p-dioxins
Hexachlorinated dibenzofurans
Heptachlorinated dibenzo-p-dioxins
Heptachlorinated dibenzofurans
Octachlorodibenzo-p-dioxin
Octachlorodibenzofurans

Organochlorine Pesticides

Hexachlorobenzene
4-4'-DDD
4-4'-DDE
4-4'-DDT
Dieldrin
Heptachlor
Heptachlor epoxide
Alpha-chlordane
Gamma-BCH (Lindane)
Gamma-chlordane
Endrin
Endrin Ketone
Toxaphene

Phenoxy Herbicides

2,4-D
2,4-DB
2,4,5-T
2,4,5-TP

Organophosphate Pesticides

Malathion
Parathion

Metals

Arsenic
Barium
Berylium
Cadmium
Chromium
Copper
Mercury
Nickel
Lead
Manganese
Selenium
Zinc
Vanadium

Acids

Hydrochloric acid
Sulfuric acid
Chromic acid
Nitric acid

Bases

Sodium hydroxide
Calcium hydroxide
Potassium hydroxide

Polychlorinated Biphenyls

Aroclor 1248
Aroclor 1260
Aroclor 1254
Aroclor 1242

Phenols

Phenol
2-4-dimethylphenol
4-methylphenol

Monocyclic Aromatic Compounds

Benzene
Ethylbenzene

Toluene
Xylenes (total)

Polycyclic Aromatic Hydrocarbons

2-Methylnaphthalene
Acenaphthene
Acenaphthalene
Anthracene
Benzo[a]anthracene
Benzo[b]fluoranthene
Benzo[ghi]prylene
Benzo[k]fluoranthene
Chyrsene
Dibenz[a,h]anthracene
Fluoranhene
Fluorene
Ideno[1,2,3]pyrene
Naphthalene
Phenanthrene
Pyrene

Glycol Ethers

2-methoxyethanol acetate
2-methoxymethanol
2-Butoxyethanol (Ethylene glycol monobutyl ether, Butyl CellosolveR)
2-2'Ethylmedioxybis(ethanol) (Triethylene glycol)
1-Ethoxy-2-(2-ethylethoxy)ethane (Diethylene glycol diethyl ether, Diethyl CarbitolR)
2-Phenoxyethanol
2-Phenoxethoxyethanol
1-(2-methoxy-1-methylethoxy)-2-propanol
1-(2-methoxypropoxy)-2-propanol
1-(2-(methoxy-1-methylethoxy)-2)-1-methlethoxy)-2-propanol

Alcohols

Methanol
Elthanol
2-Methyl-1-propanol
2-Ethyl-1-hexanol

Appendix B--Example for the Selection of Indicator Chemicals for One Medium

Chemicals Detected	Frequency of Detection	Maximum Concentration (ug/liter)
Chloromethane	6/50	1
Di(2ethylhexyl)phthalate (DEHP)	17/50	0.7
Methylene chloride	15/50	12
Naphthalene	8/50	1
Trichlorofluoromethane	6/50	3
1,1 Dichloroethane	38/50	222
Unidentified glycol ethers	30/50	7
Benzene	7/50	21
1,2 Dichloroethane	35/50	351
2,4 Dimethylphenol	6/50	45
1,1,1 Trichloroetane	26/50	420
Ethylbenzene	11/50	7
1,1,2 Trichloroethane	6/50	0.2
Toluene	13/50	1
Cis-Dichloroethylene	6/50	16
Phthalate esters (unidentified)	11/50	2.4
Trans-dichloroethylene	17/50	28
2-Methoxy ethanol	6/50	12
Xylenes	10/50	7
Pentachlorophenol	16/50	8
Trichloroethylene	27/50	7
Acetone	11/50	140
Carbon tetrachloride	8/50	3
2-Phenoxyethanol	17/50	10
Vinyl chloride	19/50	14
Methyl ethyl ketone	17/50	4
Tetrachloroethylene	37/50	89
Phenol	1/50	11
Benzo[a]pyrene	3/50	0.3
Fluorene	6/50	0.1
Propylene glycol monoethylether	2/50	1
2-Ethoxyethanol	17/50	10
Isopherone	6/50	3
Methylisobutyl ketone	9/50	9
Dimethyl phthalate	6/50	0.1
Diethyl phthalate	11/50	0.4
Butyl benzyl phthalate	7/50	0.1
2-Methoxyethanol acetate	3/50	3

Medium-Ground Water

Chemicals Detected	Frequency of Detection	Maximum Concentration (ug/liter)
Halogenated C1 and C2 Compounds		
Methylene chloride	15/50	12
Trichlorofluoromethane	6/50	3
1,2-Dichloroethane	35/50	351
1,1,1-Trichloroethane	26/50	420
1,1,2-Trichloroethane	6/50	0.2
Cis-dichloroethylene	6/50	16
Trans-dichloroethylene	17/50	28
Trichloroethylene	27/50	7
Carbon tetrachloride	8/50	3
Vinyl chloride	19/50	14
Tetrachloroethylene	37/50	89
Dibromochloropropane	7/50	1
Ketones		
Acetone	11/50	140
Methyl ethyl ketone	17/50	46
Isophorone	6/50	3
Methyl isobutyl ketone	9/50	9
Phthalates		
Di(2ethylhexyl)phthalate (DEHP)	17/50	0.7
Dimethyl phthalate	6/50	0.1
Diethyl phthalate	11/50	0.4
Butyl benzyl phthalate	7/50	0.1
Phthalate esters (unidentified)	31/50	2.4
Glycol Ethers		
2-Methoxyethanol	6/50	12
2-Ethoxyethanol acetate	13/50	30
2-Ethoxyethanol	17/50	10
2-Methoxyethanol acetate	3/50	3
Propylene glycol monomethyl ether	2/50	1
Unidentified glycol ethers	30/50	7
Monocyclic Aromatics		
Benzene	7/50	21
Ethylbenzene	11/50	7
Toluene	13/50	1

Xylenes	10/50	7
Phenols		
Pentachlorophenol	16/50	8
Phenol	1/50	11
2,4-Dimethylphenol	6/50	5
Polycyclic Aromatic Hydrocarbons		
Naphthalene	8/50	1
Fluorene	6/50	0.1
Benzo[a]pyrene	3/50	0.3

MEDIUM: WATER CHEMICAL CLASS: CARCINOGENS

Chemicals	Concentration (mg/liter)	EPA Classification	Oral Cancer a/ Potency (mg/kg-day)-1
Halogenated C1 and C2 Chemicals			
Dibromochloropropane	0.001	B2	7
Methylene chloride	0.012	B2	0.003
1,2-Dichloroethane	0.351	B2	0.07
1,1,2-Trichloroethane	0.0002	C	0.057 b/
Trichloroethylene	0.007	B2	0.015
Carbon tetrachloride	0.003	B2	0.15
Tetrachloroethylene	0.089	B2	0.051
Vinyl chloride	0.014	A	0.27
Phthalates			
Di(2-ethylhexyl) phthalate	0.0007	B2	0.0084
Unidentified phthalate esters	0.0024	B2c/	0.0084 c/
Monocyclic Aromatic Hydrocarbons			
Benzene	0.021	A	0.1
Phenols			
Pentachlorophenol	0.008	B2	0.018
Polycyclic Aromatic Hydrocarbons			
Benzo[a]pyrene	0.0003	B2	12

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a/ Cal/EPA values unless otherwise noted.
b/ Value from EPA HEAST 1991.
c/ Since the identity of these substances is unknown, they are assigned EPA carcinogen classification and oral potency values equivalent to the most potent chemical within the phthalate ester chemical class.

MEDIUM: WATER CHEMICAL CLASS: CARCINOGENS

Chemicals	IICSC	(IICSC/TICSC) x 100
Halogenated C1 and C2 Chemicals		
Dibromochloropropane	0.007	15.1
Methylene chloride	0.000042	0.0009
1,2-Dichloroethane	0.025	53.0
1,1,2-Trichloroethane	0.000011	0.025
Trichloroethylene	0.000105	0.23
Carbon tetrachloride	0.00045	0.97
Tetrachloroethylene	0.00454	9.80
Vinyl chloride	0.00378	8.16
Phthalates		
Di(2-ethylhexyl) phthalate	0.000006	0.013
Unidentified phthalate esters	0.000020	0.044
Monocyclic Aromatic Hydrocarbons		
Benzene	0.0021	4.53
Phenols		
Pentachlorophenol	0.000144	0.31
Polycyclic Aromatic Hydrocarbons		
Benzo[a]pyrene	0.0036	7.80

IICSC = Individual Indicator Chemical Score for Carcinogens
TICSC = Total Indicator Chemical Score for Carcinogens (TICSC) = 0.04634.

MEDIUM: WATER CHEMICAL CLASS: CARCINOGENS

CARCINOGENS SELECTED FOR THE QUANTITATIVE RISK ASSESSMENT

Chemicals	**(IICSC/TICSC) x 100**
Halogenated C1 and C2 Chemicals	
Dibromochloropropane	15.1
1,2 Dichloroethane	53.0
Tetrachloroethylene	9.80
Vinyl chloride	8.16
Phthalates	
Di(2-ethylhexyl) phthalate	0.013
Unidentified phthalate esters	0.044
Monocyclic Aromatic Hydrocarbons	
Benzene	4.53
Phenols	
Pentachlorophenol	0.31
Polycyclic Aromatic Hydrocarbons	
Benzo[a]pyrene	7.80
TOTAL	98.75

IICSC = Individual Indicator Chemical Score for Carcinogens.
TICSC = Total Indicator Chemical Score for Carcinogens.

MEDIUM: WATER CHEMICAL CLASS: NON-CARCINOGENS

Chemicals	Concentration (mg/liter)	Oral RfD a/	IICSNC	(IICSNC/TICSNC) x 100
Halogenated C1 and C2 Chemicals				
Trichlorofluromethane	0.003	0.3	0.001	0.004
1,1,1-Trichloroethane	0.42	0.09	4.67	19.74
Cis-dichloroethylene	0.016	0.001	1.6	6.8
Trans-dichloroethylene	0.028	0.02	1.4	5.9
Ketones				
Acetone	0.14	0.1	1.4	5.9
Methyl ethyl ketone	0.046	0.05	0.92	3.9
Isophorone	0.003	0.2	0.15	0.063
Methyl isobutyl ketone	0.009	0.05	0.18	0.76
Phthalates				
Dimethyl phthalate	0.0001	1.0	0.0001	0.004
Diethyl phthalate	0.0004	0.8	0.0005	0.002
Butyl benzyl phthalate	0.0001	0.20	0.0005	0.002
Glycol Ethers				
2-Methoxyethanol	0.012	0.004	3.0	12.68
2-Ethoxyethanol acetate	0.03	0.3	0.1	0.42
2-Ethoxyethanol	0.01	0.4	0.025	0.11
2-Methoxyethanol acetate	0.003	0.002	1.5	6.3
Propylene glycol mono methyl ether	0.001	0.7	0.0014	0.006
Unidentified glycol ethers	0.007	0.002 b/	3.5	14.79

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a/ Values from EPA IRIS or EPA HEAST unless otherwise noted.

b/ Since the identity of these substances is unknown, they are assigned an EPA classification and oral reference dose equivalent to the most potent chemical within the glycol ether chemical class

IICSNC = Individual Indicator Chemical Score for NonCarcinogens

TICSNC = Total Indicator Chemical Score for NonCarcinogens (TICSNC) = 23.66

Monocyclic Aromatic Hydrocarbons				
Ethylbenzene	0.007	0.1	0.07	0.30
Toluene	0.001	0.2	0.005	0.02
Xylenes (mixed)	0.007	2.0	0.0035	0.015
Phenols				
Phenol	0.011	0.60	0.018	0.08
2,4 Dimethylphenol	0.005	0.001	5.0	21.13
Polycyclic Aromatic Hydrocarbons				
Naphthalene	0.001	0.004	0.25	1.1
Fluorene	0.0001	0.04	0.0025	0.011

MEDIUM: WATER CHEMICAL CLASS: NON-CARCINOGENS

NON-CARCINOGENS SELECTED FOR THE QUANTITATIVE RISK ASSESSMENT

Chemicals	**(IICSNC/TICSNC) x 100**
Halogenated C1 and C2 Chemicals	
1,1,1-Trichloroethane	19.74
Cis-dichloroethylene	6.8
Trans-dichloroethylene	5.9
Ketones	
Acetone	5.9
Methyl ethyl ketone	3.9
Phthalates	
Diethyl phthalate	0.002
Glycol Ethers	
2-Methoxyethanol	12.68
2-Methoxyethanol acetate	6.3
Unidentified glycol ethers	14.79
Monocyclic Aromatic Hydrocarbons	
Ethylbenzene	0.30
Phenols	
2,4-Dimethylphenol	21.13
Polycyclic Aromatic Hydrocarbons	
Naphthalene	1.1
TOTAL	98.5

MEDIUM: WATER CHEMICAL CLASS: ALL

CHEMICALS SELECTED FOR THE QUANTITATIVE RISK ASSESSMENT

Halogenated C1 & C2 Chemicals
Dibromochloropropane
1,2-Dichloroethane
Tetrachloroethylene
Vinyl chloride
1,1,1-Trichloroethane
Cis-dichloroethylene
Trans-dichloroethylene

Phthalates
Di(2-ethylhexyl) phthalate
Unidentified phthalate esters
Diethyl phthalate

Monocyclic Aromatic Hydrocarbons
Benzene
Ethylbenzene

Phenols
Pentachlorophenol
2,4-Dimethylphenol

Polycyclic Aromatic Hydrocarbons
Benzo[a]pyrene
Naphthalene

Ketones
Acetone
Methyl ethyl ketone

Glycol Ethers
2-Methoxyethanol
2-Methoxyethanol acetate
Unidentified glycol ethers

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